Density Matrix Renormalization Group and the Nuclear Shell Model

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(Dated: February 9, 2008)

We describe the use of the Density Matrix Renormalization Group method as a means of approximately solving large-scale nuclear shell-model problems. We focus on an angular-momentum-conserving variant of the method and report test results for the nucleus ^{48}Cr. The calculation is able to reproduce both the ground state energy and the energy of the first excited state, by diagonalizing matrices much smaller than those of the full shell model.

PACS numbers: 21.60.Cs, 05.10.Cc

I. INTRODUCTION

In the traditional nuclear shell model [1], the low-energy structure of a given nucleus is described by assuming an inert doubly–magic core and then diagonalizing the effective nuclear hamiltonian within an active valence space consisting of at most a few major shells. Despite the enormous truncation inherent in this approach, the shell-model method as just described can still only be applied in very limited nuclear regimes, namely for those nuclei with a sufficiently small number of active nucleons or a relatively low degeneracy of the valence shells that are retained. For heavier nuclei or nuclei farther from closed shells, one must truncate further to reduce the number of shell-model configurations to a manageable size.

An attractive truncation possibility is provided by the Density Matrix Renormalization Group (DMRG), a method initially developed for low-dimensional quantum lattices [2]. Subsequently, the method was extended to finite Fermi systems and applied to ultrasmall superconducting grains [3], to problems in quantum chemistry [4] and to two-dimensional electrons in strong magnetic fields [5]. The great success of these applications suggests that it could also prove useful for obtaining accurate approximate solutions to the nuclear shell model, in cases where exact diagonalization is not feasible.

The DMRG method involves a systematic inclusion of the degrees of freedom of the problem. When treating quantum lattices, real-space sites are added iteratively. In finite Fermi systems, these sites are replaced by single-particle levels. At each stage, the system [referred to as a *block*] is enlarged to include the additional site or level. This enlarged block is then coupled to the rest of the system (the *medium*) giving rise to the *superblock*. For a given eigenstate of the superblock (often the ground state) or perhaps for a group of important eigenstates, the reduced density matrix of the enlarged block in the presence of the medium is constructed and diagonalized and those states with the largest eigenvalues are retained. This method of truncation is guaranteed to be optimal in the sense that it maximizes the overlap of the approximate (truncated) wave function with the targeted superblock wave function prior to truncation.

The earliest application of the DMRG method in the context of nuclear structure was based on the use of a particle-hole variant of the method [6]. In this approach, the group of single-particle levels was divided into four subgroups, neutron particle, neutron hole, proton particle and proton hole. The results of those calculations were not terribly encouraging, however, as they required that a substantial fraction of the full shell model space be retained for a reasonable reproduction of the results from exact diagonalization.

More recently a more traditional DMRG study was reported that did not adopt the particle-hole strategy [7]. The method worked extremely well for the nucleus ^{28}Si, giving an accurate reproduction of the exact shell-model results with a significantly reduced basis. In contrast, the results for ^{56}Ni were not nearly as good, as the method seemed to be converging to a solution energetically still far from the exact ground state.

One of the limitations of the above studies is that they did not preserve symmetries throughout the iterative inclusion of single-particle levels. Since the density matrix procedure involves a truncation at each of the iterative stages, there is a potential to lose these symmetries and the associated correlations. In such cases, the iterative procedure must incorporate not only dynamical correlations but also the kinematical correlations associated with symmetry restoration.

This point has been recognized for some time in DMRG applications outside the nuclear domain. McCulloch and Gulácsi [8] discussed how to reformulate the DMRG to maintain symmetries throughout. They referred to this as the non-Abelian DMRG method and showed that it could produce more accurate results than the traditional Abelian method while using smaller spaces.

In this work, we adopt a strategy whereby angular momentum is preserved throughout the iterative DMRG process. We refer to this as the JDMRG method. It was briefly described as part of a recent review [9]. Subse-

quently, the method was applied in nuclear physics for the first time in the context of the Gamow Shell Model [10].

An outline of the paper is as follows. In Sec. II, we provide a brief overview of the traditional Abelian DMRG method and then in Sec. III describe the modifications required to maintain rotational invariance as an exact symmetry. In Sec. IV, we briefly review the test problem we treat and describe in some detail our implementation of the JDMRG method for this problem. Section V describes our results. Section VI summarizes the principal conclusions reached in this study and outlines directions for future work.

II. OVERVIEW OF THE DMRG METHOD

We begin by describing the traditional Abelian DMRG method, as has been used in almost all applications to date. We focus on finite Fermi systems, for which the degrees of freedom being systematically incorporated by the method are single-particle levels.

Assume we have treated a set of L levels and that the total number of states we have kept to describe that *block* is m.

We now add the next level, the $L+1^{st}$, which admits s states. In the traditional DMRG approach, the states we build in the enlarged block are simply products of those in the original block and in the extra level. Thus, when we enlarge the block to include the $L+1^{st}$ level, it results in a new block with $m \times s$ states.

Renormalization Group methods, whether Wilson's original numerical algorithm or White's Density Matrix version, then implement a truncation of the states of the enlarged block to the same number m as before the block enlargement.

In Wilson's numerical RG procedure, the truncation involves diagonalizing the hamiltonian in the $m \times s$-dimensional space of the enlarged block and retaining its lowest m eigenstates.

In White's DMRG approach, the truncation is implemented through a very different procedure, schematically illustrated in figure 1. Consider the enlarged block B' (the block B plus the added level) in the presence of a medium M that approximates the rest of the system. White's truncation is carried out based on the importance of the block states in a selected set of target states of the full *superblock*, *i.e.,* the eigenstates of B' coupled to M.

Assume here that we target only the ground state of the superblock in the truncation,

$$|\Psi_{gs}\rangle = \sum_{i=1,\ m\times s} \ \sum_{j=1,\ t} \Psi_{ij}\ |i\rangle_B\ |j\rangle_M\ , \qquad (1)$$

obtained by constructing and then diagonalizing the superblock hamiltonian. Here $|i\rangle_B$ refers to a state in the block and $|j\rangle_M$ to a state in the medium. Furthermore, t denotes the number of states of the medium. If we construct the ground-state density matrix for the enlarged block,

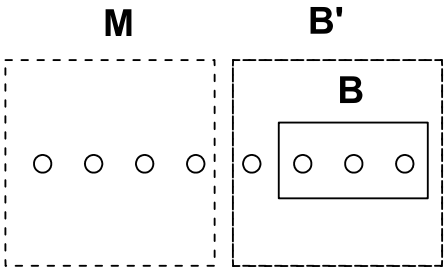

FIG. 1: Schematic illustration of the DMRG growth procedure, in which a block B is enlarged to B' in the presence of a medium M.

$$\rho^B_{ii'} \ = \ \sum_{j=1,\ t} \Psi^*_{ij}\Psi_{i'j}\ , \qquad (2)$$

diagonalize it, and truncate to the m states with the largest density-matrix eigenvalues, we are guaranteed to achieve the optimal approximation to the superblock ground state.

To target a group of states, we would construct a mixed density matrix containing information on the block content of all of them. For example, if we wished to target both the ground state and the first excited state, weighting them equally, we would construct

$$\rho^B_{ii'} \ = \ \frac{1}{2}\left(\sum_{j=1,\ t} \Psi^*_{ij}\Psi_{i'j} \ + \ \sum_{j=1,\ t} \Phi^*_{ij}\Phi_{i'j}\right), \qquad (3)$$

where Ψ as above refers to the ground state wave function and Φ correspondingly to the wave function of the first excited state.

Truncation to the most important m states in the enlarged block is accompanied by the renormalization of all operators for use in the truncated space. If the eigenstates $|\alpha\rangle$ associated with the m lowest density matrix eigenvalues are

$$|\alpha\rangle = \sum_{i=1,m\times s} c^\alpha_i|i\rangle \quad , \quad \alpha = 1, ..., m\ , \qquad (4)$$

then the matrix elements of any operator O must be renormalized according to

$$\langle\alpha|O|\beta\rangle = \sum_{i,j} c^{\alpha *}_i c^\beta_j\ \langle i|O|j\rangle\ . \qquad (5)$$

A key step in the growth procedure is to calculate at each step the matrix elements of all necessary suboperators of the hamiltonian and to store them. This includes all one- and two-point operators,

$$a^\dagger_i,\ a^\dagger_i a_j,\ a^\dagger_i a^\dagger_j,\ + h.c., \qquad (6)$$

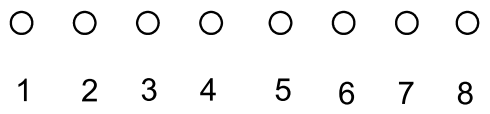

FIG. 2: Schematic illustration of the ordering of levels (or sites) in a chain to be systematically included in the DMRG growth procedure.

and all three- and four-point operators required to build the hamiltonian matrix,

$$\hat{O}^1_k = \frac{1}{4}\sum_{ijl} V_{ijkl} a^\dagger_i a^\dagger_j a_l \ + h.c. \ ,$$

$$\hat{O}^2 = \frac{1}{4}\sum_{ijkl} V_{ijkl} \ a^\dagger_i a^\dagger_j a_l a_k \ , \tag{7}$$

where $V_{ijkl} = \langle ij|V|kl\rangle$. Having this information for the block and the additional level enables it to be calculated for the enlarged block.

As an example, consider the one-body operator $a^\dagger_\alpha a_\beta$. Its matrix elements in the enlarged product space $|i,j\rangle = |i\rangle|j\rangle$, where $|i\rangle$ belongs to block B_1 and $|j\rangle$ belongs to B_2, are given by

$$\begin{aligned}\langle i,j|a^\dagger_\alpha a_\beta|k,l\rangle \ &= \ \langle i|a^\dagger_\alpha a_\beta|k\rangle \ \delta_{jl} \\ &+ \ \langle j|a^\dagger_\alpha a_\beta|l\rangle \ \delta_{ik} \\ &+ \ (-)^{n_k}\langle i|a^\dagger_\alpha|k\rangle \ \langle j|a_\beta|l\rangle \\ &- \ (-)^{n_k}\langle i|a_\beta|k\rangle \ \langle j|a^\dagger_\alpha|l\rangle \ , \end{aligned} \tag{8}$$

where n_i is the number of particles in state $|i\rangle$. Note that the matrix elements of a two-point operator in the product space is expressed in terms of matrix elements of one- and two-point operators in the spaces of the two component blocks.

We now have the basic tools in hand to discuss how the traditional DMRG procedure is implemented. It involves a series of steps. The first is to choose an active space and a hamiltonian to act in that space. Next we choose an order in which the single-particle levels are included. Typically, this is done by organizing the levels in a chain, as schematically illustrated in figure 2.

The following step is usually referred to as the warmup phase. This step involves making an initial guess for the optimal structure in each size block for a given choice of the number of retained states m. For the eight levels shown in figure 2, we would make a first guess at the structure of the blocks $B(1,2)$, $B(1,3)$, $B(1,4)$, $B(1,5)$, $B(1,6)$, $B(1,7)$ and $B(1,8)$. Having a guess for the optimal m states in each block, we can calculate (and store) all the necessary matrix elements in those truncated blocks. The warmup guess can be implemented in a variety of ways, depending on the specific problem.

The next step, and indeed the heart of the DMRG method, is the sweep phase, which we now describe by focusing again on the chain of eight levels in figure 2.

We begin the sweep phase by growing level 8 into a two-level block $B(7,8)$. To determine the optimal m states in that enlarged block, we immerse it in a medium consisting of the block $B(1,6)$ from the warmup phase. We diagonalize the superblock hamiltonian for the full system, then calculate the reduced density matrix associated with the enlarged block, and renormalize all operators to act in the truncated space associated with the m largest eigenvalues.

We then continue the process, enlarging to $B(6,8)$, immersing it in a medium consisting of $B(1,5)$ and then truncating and renormalizing $B(6,8)$ based on its reduced density matrix eigenvalues.

This process is continued until all size blocks have been treated.

At this point, we simply reverse the direction of the sweep, now growing the system from left to right, always treating the enlarged block in a medium consisting of the rest of the levels as obtained in the previous sweep. This process is continued until acceptably small changes from one sweep to the next are achieved. At this point, we have hopefully arrived at an optimal block structure and an optimal description of the system for the assumed value of m.

The calculation is then carried out as a function of m, until acceptably small changes with increasing values are achieved. At this point, we hopefully have a good approximation to the exact solution of the problem. Obviously, the solution is especially useful if this good approximation can be achieved while retaining only a small fraction of the full Hilbert space.

III. THE JDMRG METHOD

We now describe the modifications to the traditional DMRG algorithm required to preserve rotational symmetry throughout.

As noted earlier, the DMRG systematically grows the system by adding additional degrees of freedom. This is most conveniently accomplished by adding doubly-degenerate levels, either Nilsson-like levels or the $+m$ and $-m$ levels of an nlj multiplet. A great advantage of this is that every level looks very similar to every other, greatly simplifying the algorithm by which they are computationally included.

In the JDMRG, it is essential that throughout the procedure the states have definite angular momentum. To accomplish this, it is critical that we add at each stage states of definite angular momentum. This is most

readily accomplished by always adding a complete shell, rather than a partial shell or a non-spherical single-particle level.

The goal of a calculation is to construct and diagonalize the hamiltonian in the the space in which all levels have been included. As noted earlier, the traditional DMRG works in a product (or m-scheme) representation. In this case, we need to build the matrix elements of all hamiltonian sub-operators directly in the m-scheme, as this is what is needed to build the matrix elements in the enlarged system and ultimately the matrix elements of the superblock hamiltonian. For each size block those m-scheme matrix elements must then be stored, for use in the following sweep.

In an angular-momentum-conserving approach we must instead calculate and store throughout the iterative process the *reduced matrix elements* of all relevant sub-operators of the hamiltonian, namely

$$a_i^\dagger,\ [a_i^\dagger \tilde{a}_j]^K,\ [a_i^\dagger a_j^\dagger]^K,$$

$$\begin{aligned}
\hat{O}^1_l = -\sum_{ijkK} \quad & \sqrt{(1+\delta_{ij})(1+\delta_{kl})}\ \hat{K}\ V^K_{ijkl} \\
\times \quad & \left([a_i^\dagger a_j^\dagger]^K \tilde{a}_k\right)^l , \\
\hat{O}^2 = -\sum_{ijklK} \quad & \sqrt{(1+\delta_{ij})(1+\delta_{kl})}\ \hat{K}\ V^K_{ijkl} \\
& \times \left([a_i^\dagger a_j^\dagger]^K\ [\tilde{a}_k \tilde{a}_l]^K\right)^0 , \qquad (9)
\end{aligned}$$

and the relevant hermitean conjugates. Here, $\hat{K} = \sqrt{2K+1}$, $\tilde{a}_{jm} = (-)^{j-m} a_{j-m}$ and

$$V^K_{ijkl} = \langle ij(K)|V|kl(K)\rangle.$$

As an illustration of how this proceeds, consider the reduced matrix elements of the coupled one-body operator $[a_i^\dagger \tilde{a}_j]^K$ in an enlarged space obtained by coupling blocks B_1 and B_2. Denoting the coupled states as $|\alpha K, \beta L(J)\rangle$, where $|\alpha K\rangle$ refers to the state in B_1, $|\beta L\rangle$ to the state in B_2, and J to the coupled angular momentum, the matrix elements are given by

$$\begin{aligned}
&\langle \alpha' K', \beta' L'(J') || [a_i^\dagger \tilde{a}_j]^\lambda || \alpha K, \beta L(J)\rangle \ = \\
&\quad \delta_{\beta\beta'}\delta_{LL'}\,(-)^{K'+L'+J+\lambda}\ \widehat{J}\widehat{J'} \begin{Bmatrix} K' & J' & L' \\ J & K & \lambda \end{Bmatrix} \\
&\quad \times \langle \alpha' K' \| \left(a_i^\dagger \tilde{a}_j\right)^\lambda \| \alpha K\rangle + \\
&\quad + \delta_{\alpha\alpha'}\delta_{KK'}\,(-)^{K'+L+J'+\lambda}\ \widehat{J}\widehat{J'} \begin{Bmatrix} L' & J' & K' \\ J & L & \lambda \end{Bmatrix} \\
&\quad \times \langle \beta' L' \| \left(a_i^\dagger \tilde{a}_j\right)^\lambda \| \beta L\rangle + \\
&\quad + (-)^{n_{\alpha K}}\ \widehat{J}\widehat{J'}\widehat{\lambda} \begin{Bmatrix} K' & L' & J' \\ K & L & J \\ i & j & \lambda \end{Bmatrix} \\
&\quad \times \langle \alpha' K' \| a_i^\dagger \| \alpha K\rangle \times \langle \beta' L' \| \tilde{a}_j \| \beta L\rangle + \\
&\quad + (-)^{i-j+\lambda}\ \ (-)^{n_{\alpha K}}\ \widehat{J}\widehat{J'}\widehat{\lambda} \begin{Bmatrix} K' & L' & J' \\ K & L & J \\ j & i & \lambda \end{Bmatrix} \\
&\quad \times \langle \alpha' K' \| \tilde{a}_j \| \alpha K\rangle \times \langle \beta' L' \| a_i^\dagger \| \beta L\rangle \ , \qquad (10)
\end{aligned}$$

where $n_{\alpha K}$ is the number of particles in state $|\alpha K\rangle$. Knowing the reduced matrix elements of the one- and two-point operators $a_i^\dagger,\ [a_i^\dagger \tilde{a}_j]^K,\ [a_i^\dagger a_j^\dagger]^K$ in the two component blocks enables us to determine the reduced matrix element of interest for the enlarged block.

Otherwise, the JDMRG involves the same set of basic steps as the traditional DMRG.

IV. THE TEST MODEL

The test results we report in this paper are for the nucleus ^{48}Cr, treated as four valence neutrons and four valence protons outside doubly-magic ^{40}Ca. We restrict both the valence neutrons and the valence protons to the orbits of the $1f2p$ shell. Furthermore, we use in these calculations the shell model hamiltonian KB3, for which exact results are available. The size of the full space for ^{48}Cr is 1,963,461 states. Of these, 41,355 are 0^+ states, 182,421 are 2^+ states, etc.

A. Some specifics of our implementation for this test problem

In the calculations reported here, we separate neutron from proton orbitals, rather than putting them in a single chain. As we will soon see, this leads to a three-block strategy for implementing the JDMRG truncation.

With that as background, we now describe how we implement the two stages of the analysis, the warmup stage and the sweeping stage, for the ^{48}Cr test problem we have considered.

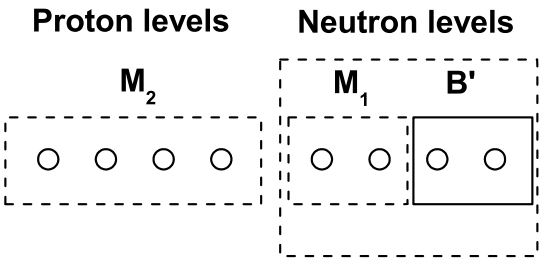

FIG. 3: Schematic illustration of the three-block sweeping strategy used in the calculations reported herein. The enlarged neutron block B' is immersed in a medium consisting of the remaining neutron levels (block M_1) and all the proton levels (block M_2).

1. Warmup

As noted earlier, the initial warmup stage of the DMRG procedure involves choosing a first approximation to the optimal truncated structure of each group of single-particle levels. Because of our separation of neutrons from protons, the groups of relevance are groups of neutron orbits and separately groups of proton orbits. Labelling the four orbits as $1 \to 4$ (note that we have not yet defined the order of the four active orbits), we need information on the following blocks: $B(1,2)$, $B(1,3)$, $B(1,4)$. While we need them for both neutrons and protons, the symmetry of the problem allows us to choose them the same for both.

Our procedure is to gradually build the identical orbit block, by systematically adding orbit $i+1$ to the block $B(1,i)$. At each stage of the warmup growth, we construct a *superblock* by coupling the enlarged neutron block to the corresponding enlarged proton block (*i.e.,* the block with the same set of orbits). We construct the superblock for N=Z, from $0 \to 4$, and for $J^\pi = 0^+$. Targeting the ground state for each of these N=Z systems, we obtain the corresponding reduced density matrices and implement our truncation.

The truncation is carried out to those m states with the largest density matrix eigenvalues. We do not worry about making sure that at least one state is kept for each $N(or\ Z)$ and J, as our experience in *these* calculations indicates it is not necessary.

2. Sweeping

As noted earlier, our procedure of separating neutron from proton orbitals, rather than lining them up in a single chain, gives rise to a three-block strategy in the sweeping process. We now expand on what is meant by this, by reference to figure 3.

Let us assume that we are growing the system for one type of particle (neutrons, for specificity), building from a block B to an enlarged block B'. The medium in which we carry out the truncation of that enlarged block includes two components. One component, denoted M_1 in the figure, involves the rest of the neutron orbits, for which the corresponding optimal structure was defined in the previous sweep (or in the warmup phase). The second component, denoted M_2 in the figure, involves *all* of the orbits of the protons, for which likewise the optimal structure was obtained in the previous stage. Put another way, the states in the superblock have the form

$$\left| \left\{ \left[(n_\nu \alpha_\nu J_\nu)\, (4 - n_\nu\ \alpha'_\nu J'_\nu) \right]^{J_\pi} (4\ \beta_\pi J_\pi) \right\}_{M=0}^{L=0} \right\rangle \ ,$$

with n_ν neutrons in the enlarged neutron block B', $4-n_\nu$ neutrons in M_1 and 4 protons in M_2.

By diagonalizing the hamiltonian in that basis, we arrive at a ground state wave function

$$|L=0\ G.S.\rangle = \sum_{\alpha_\nu J_\nu \alpha'_\nu J'_\nu \beta_\pi J_\pi K_\nu} X_{\alpha_\nu J_\nu \alpha'_\nu J'_\nu \beta_\pi J_\pi} \times \left| \left\{ \left[(n_\nu \alpha_\nu J_\nu)\, (4 - n_\nu\ \alpha'_\nu J'_\nu) \right]^{J_\pi} (4\ \beta_\pi J_\pi) \right\}_{M=0}^{L=0} \right\rangle , \tag{11}$$

from which the reduced density matrix associated with B' can be readily evaluated and then diagonalized for each n_ν and J_ν. Truncation to the m states with the largest density matrix eigenvalues gives the optimal structure of the truncated block B', which is stored for use in the next sweep stage.

3. The whole process

We now have in hand all that is needed to fully describe our calculational algorithm. It involves the following steps.

1. Order the single-particle states. Indeed, in the results we will report, we simply use the ordering $p_{1/2}$, $p_{3/2}$, $f_{5/2}$, $f_{7/2}$ in terms of increasing angular momentum, with no effort at optimization.

2. For each m, we carry out the warmup as prescribed in Sec. IV A storing the results (*i.e.,* the reduced matrix elements) for each group of orbits.

3. We then begin by sweeping downwards through the orbits, growing from orbit 4 to a block $B(4,3)$. The medium for implementing this truncation involves the block $B(1,2)$ for the same type of particle and the block $B(1,4)$ for the other, both of which were obtained either in the warmup or in the previous sweep.

4. We iterate the above step until all sets of orbits have been treated.

5. We then reverse and begin sweeping upwards, growing the block and implementing a truncation based on its coupling to the other two relevant blocks.

6. We view a sweep down and the following sweep up as a single sweeping stage. It involves six growing steps, each one giving a ground state eigenvalue. We denote the lowest of these six eigenvalues by E^n_{min}, where n denotes the sweeping stage number.

7. As we systematically sweep up and down, we compare E^n_{min} with E^{n-1}_{min}, *i.e,* we look at the change in the minimum energy from one sweeping stage to the next. When this change is sufficiently small, typically of order 10^{-4} MeV, we stop the calculation. No more than 7 sweeping stages were required to achieve this level of convergence in any of the calculations we carried out.

8. We then increment m and repeat the set of steps $2 \rightarrow 7$.

V. RESULTS

Our results for the ground state are presented in table 1. The exact calculation produces a ground state energy of -32.95 MeV. The DMRG calculation with $m = 50$ produces a result of -32.80 MeV, about 150 keV from the exact result. In this case, the largest matrix that had to be diagonalized had a dimension of 3,657. The conclusion is that the three-block JDMRG algorithm gives a good reproduction of the exact results for the ground state with a fairly small number of states retained in each block, but by calculating matrices with a substantial fraction (roughly 8-9%) of the full basis.

TABLE I: Results for the ground-state energy from the JDMRG calculations described in the text. *Max Dim* refers to the maximum dimension of the hamiltonian matrix that required diagonalization.

m	E_{GS} (MeV)	$Max\ Dim$
20	-32.28	1,591
25	-32.47	1,893
30	-32.57	2,327
35	-32.66	2,685
40	-32.72	3,109
45	-32.76	3,403
50	-32.80	3,657
$Exact$	-32.95	41,355

For any value of m, we can calculate excitation energies as well, by working in spaces that are based on the optimized blocks. As a reminder, during the sweep procedure we diagonalize the superblock hamiltonian in a basis in which all states of the added level are included. Following the density-matrix-based truncation, the enlarged block has fewer states, and often significantly fewer. It is in this reduced space that we can recalculate the ground state, by diagonalizing in the truncated 0^+ space, and also carry out diagonalizations for other angular momenta. The results for $m = 50$ are illustrated in table 2, for the excitation energies of the lowest 2^+, 4^+ and 6^+ states. The result for the lowest 2^+ state is in quite good agreement with the exact result, despite the diagonalization of a matrix that is less than 5% of the full matrix. For the 4^+ and 6^+ states, the results remain fairly good, although progressively worse than for the lower J values. These results can of course be improved by further increasing m. Overall, we conclude that the method seems capable of producing reasonable results for low-lying excited states as well, even when we target the ground state only.

TABLE II: Results for the excitation energies of low-lying excited states from the DMRG calculations described in the text at a value of m=50. All results are in MeV.

J^π	$JDMRG$	$Exact$
2^+	0.84	0.81
4^+	2.02	1.82
6^+	3.95	3.40

VI. SUMMARY AND OUTLOOK

In this paper, we have described an approach for solving the nuclear shell-model problem in cases in which it cannot be treated by exact diagonalization. The approach makes use of the Density Matrix Renormalization Group to systematically truncate the space in which diagonalizations are carried out on the basis of well-defined dynamical considerations. The approach we develop preserves rotational symmetry throughout, to avoid losses of information associated with breaking of that critical nuclear symmetry during the truncation process.

We test these ideas in the context of a large-scale, but exactly diagonalizable, shell-model problem. Namely we apply it to the well-deformed nucleus ^{48}Cr with a realistic KB3 hamiltonian. For these test calculations, we used a three-block DMRG strategy, in which neutron and proton levels were not mixed in blocks. This leads to certain simplifications in the formalism, but at the cost of having to treat larger superblock matrices.

The calculations are able to produce a fairly accurate reproduction of the exact results for ^{48}Cr, both for the ground state and the first excited 2^+ state, both members of the ground state rotational band. It does this by retaining a fairly small number of states in each block. However, because of the three-block approach that was used, the dimensions of the superblock matrices we needed to treat were still a sizable fraction (5-10%) of the full shell-model space. Results for the lowest states of higher spins get progressively worse as the spin increases.

Our work in the future will focus on two fronts. On the one hand, we will continue to work with the three-block approach, addressing such issues as (i) the possibility of

improving convergence by altering the order in which levels are included, building on the work of Legeza and collaborators [11], and (*ii*) the possibility of speeding up the calculations by replacing m as the convergence variable by the sum of neglected density matrix eigenvalues [12]. At the same time, we are now in the process of developing a two-block JDMRG code [13], in which blocks containing both neutron and proton orbits are built. This should enable us to dramatically increase the number of states retained in a block for a given size of the full superblock matrix. This will be critical as we consider the application of these methods to heavier nuclei, the ultimate goal of the project.

Acknowledgements

This work was supported in part by the US National Science Foundation under grant # PHY-0140036. We acknowldege with deep appreciation the many contributions of Jorge Dukelsky to this project. We also thank Alfredo Poves for providing the matrix elements and exact results used in this work and Larisa Pacearescu for her contributions in the early stages. Finally, we are grateful to Ian McCulloch for valuable discussions on the non-Abelian DMRG method.

[1] *The Nuclear Shell Model*, K. Heyde, (Springer-Verlag, Berlin, 1990).
[2] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); S. R. White, Phys. Rev. **B48**, 10345 (1993).
[3] J. Dukelsky and G. Sierra, Phys. Rev. Lett. **83**, 172 (1999); J. Dukelsky and G. Sierra, Phys. Rev. **B61**, 12302 (2000).
[4] S. R. White and R. L. Martin, J. Chem. Phys. **110**, 4127 (1999); S. Daul, I. Ciofini, C. Daul, Steven R. White, Int. J. Quantum Chem. **79**, 331 (2000).
[5] N. Shibata and D. Yoshioka, Phys. Rev. Lett. **86**, 5755 (2001); D. Yoshioka and N. Shibata, Physica **E12**, 43 (2002); N. Shibata, J. Phys. A **36**, R381 (2003).
[6] S. Pittel, J. Dukelsky, S. Dimitrova and M. Stoitsov, Rev. Mex. Física **49, Supp. 4**, 82 (2003).
[7] T. Papenbrock and D. J. Dean, J. Phys. G **31**, S1377 (2005).
[8] I. McCulloch and M. Gulácsi, Europhys. Lett. **57**, 852 (2002).
[9] J. Dukelsky, and S. Pittel, Rep. Prog. Phys. **67**, 513 (2004).
[10] N. Michel, W. Nazarewicz, M. Ploszajczak and J. Rotureau, Rev. Mex. Física **50** Num. 2, 74 (2004).
[11] Ö. Legeza, J. Röder and B. A. Hess, Phys. Rev. **B67**, 125114 (2003).
[12] Ö. Legeza and J. Sólyom, Phys. Rev. **B68**, 195116 (2003).
[13] B. Thakur, S. Pittel, J. Dukelsky and N. Sandulescu, work in progress.